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Analysis of elastic properties of transversely isotropic CNT-reinforced polymers

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ABSTRACT

This paper presents a numerical approach for estimation of effective elastic properties of carbon nanotube (CNT)-reinforced polymer composites. A square representative volume element (RVE) denoting a part of continuum is considered based on the assumption of transverse isotropy of material and the fiber/matrix regions are discretized using three-dimensional solid elements. The meshed assembly with periodic boundary conditions is employed to predict the elastic properties using finite element analysis solver. Parametric studies are conducted by considering the properties of CNT fibers both as isotropic and orthotropic, that are uniformly distributed in isotropic polymer phase. The effect of interphase properties such as its stiffness and thickness on the elastic properties is also studied. Investigated results are in good agreement with those obtained from micromechanics model.

KEYWORDS

Rule of mixture;
Finite element analysis;
Transverse isotropy;
Interphase effects;
Elastic properties.

INTRODUCTION

The ability to withstand high load and need for light-weight, high strength materials emerged the advance composite system with better performance in structures and engineering applications. Recently engineers and researchers have given huge attention on carbon nanotube embedded polymer matrix composites for utilizing the remarkable properties of carbon nanotube (stiffness up to 1TPa, tensile strength of order of 100GPa and thermal conductivity up to 6000 $Wm^{-1}K^{-1}$) as reinforcement[1]. More generally matrix phase having considerably lower strength and density than the reinforcing phase, thus combination of fiber and matrix often gives rise to high stiffness to weight ratio. Exploitation of carbon nanotube and other nanostructures as filler made them promising candidate to advance composites. With global oil resources on a decline, increase in the fuel efficiency of engines has become highly desirable, thus CNT reinforced composites are expected to be adopted by automobile and aircraft manufacturing industries in production of reinforced lightweight machine elements in near future[2]. Besides these, CNT reinforced composites have multitude of applications encompassing fuel cell components, natural gas tanks, advanced marine vessels, oil field structure, sports equipment and electronic packaging applications. To accelerate structures and engineering application of these composites, cost factor and technological problems associated with the production process need to be resolved. For instance, non-uniform distribution of CNTs, poor dispersion, and low load transfer efficiency CNT to polymer matrix due to interphase, agglomerates formation due to strong van der Waals forces and high specific surface area have great impact on mechanical behaviour of CNT reinforced composite. The understanding of adverse effect of the above factors on the macroscopic properties and to overcome these problems an exhausting experimental work is needed. Several recent works[3,4] investigated mechanical properties of CNT-poly methyl-methacrylate reinforced composite using experimental and modeling technique. Besides experimental work, which is very costly but informative at the nano level, there are few modeling approaches that perform virtual design and optimization of CNT reinforced composite. The main modeling approaches that researchers have been used include: atomistic modeling[5,6], analytical modeling[7-10] and continuum modeling[11-14] approaches. Molecular Dynamics (MD) simulation, tight-binding molecular dynamics and density functional theory (DFT) are used for atomistic modeling. But MD simulation have remedy such as small time and length scale analysis and not suitable for multi-scale modeling. As analytical approaches are limited to meso/microscale, in recent scenario, researchers are using hybrid atomistic-continuum modeling. Investigation of elastic properties of composite using continuum mechanics approach, mainly in the form of Finite Element Method (FEM) have potential to deal with parametric investigations of the elastic properties of CNT-reinforced composites. Generally, CNT-reinforced composites shows orthotropic material properties at meso level, but during fabrication process, it is impossible to control the dispersion and distribution of the CNTs so precisely resulting in a random nanostructure.

Present paper deals with the prediction of the effective elastic constants of uniformly distributed CNT reinforcements in polymer with transverse-isotropic assumptions using FEM. An RVE consisting of square cross-section of polymer matrix embedded with single-walled CNTs along with an interphase between them is employed. The analyses are conducted by means of 3-D finite element model of RVE using commercial software ANSYS. In order to predict elastic moduli, RVE is loaded in axial tension separately in three directions by applying a small normal displacement at one side and fully restraining the other side. Analytical results obtained from the rule of mixtures are used to validate the data from finite element method. After validating, the model is used to investigate the effects of interphase and geometry parameters on the elastic properties.

MODELING OF COMPOSITE RVE

As in conventional composite fibers, CNT reinforcements can be considered to be uniformly distributed in the polymer matrix. Numerical homogenization gives the concept of representative volume element (RVE) for estimating the effective properties of the composite. Due to its simplicity, an RVE of square cross-section is selected to approximate the entire geometry during the analysis[15,16]. Figure 1 shows the typical RVE which is selected from a periodic composite structure.

The RVE consists of polymer matrix, an embedded full length CNT and interphase between them. An equivalent volume solid cylindrical CNT is considered for modeling the hollow cylindrical shape having thickness of 0.34nm. RVE model of square cross-section (9nm x 9nm) with 50nm length is considered. For Analytical analysis point of view rule of mixture is employed for estimating the elastic properties. Longitudinal and transverse elastic constants using rule of mixture[7,17] are:

$$\mathbf{E_{C1} = E_{cnt} V_{cnt} + E_M (1 - V_{cnt})} \quad (1)$$

$$\mathbf{E_{C2} = \frac{E_{cnt} E_M}{E_{cnt}(1 - V_{cnt}) + E_M V_{cnt}}} \quad (2)$$

And inter-laminar Poisson's ratio (ν_{C23}) and shear stress (G_{C23}) of composite have been estimated as:

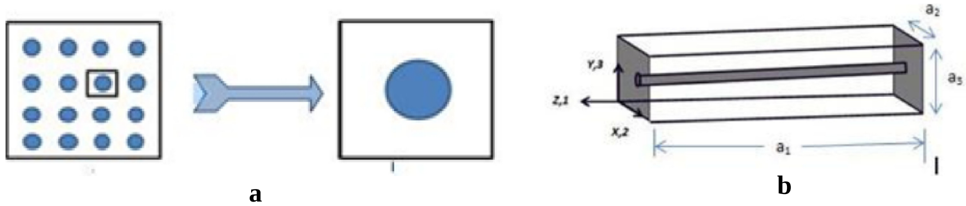


Figure1 : (a) Selected RVE from a periodic structure, (b) RVE of square section

$$\nu_{C23} = \frac{1}{\left[\frac{V_{cnt}}{\nu_{cnt}} + \frac{(1 - V_{cnt})}{\nu_M}\right]} \quad (3)$$

$$G_{C23} = \frac{E_{C2}}{2(1+\nu_{C23})} \quad (4)$$

where E_{cnt}, ν_{cnt} and E_M, ν_M are the elastic modulus, Poisson's ratio of CNT and polymer matrix respectively and V_{cnt} is CNT volume fraction.

Polymer phase

The polymer resin considered in the present investigation is Poly methyl methacrylate (PMMA). It has properties such as good impact strength, high toughness and lightweight in nature. It has various applications in primary aircraft structure, formula-1 cars and packaging. Here linear isotropic behaviour is considered with Young's modulus and Poisson's ratio of 2.5 GPa and 0.34 respectively.

Fiber phase

CNTs are hexagonal array structure in cylindrical tube form. In present task, both isotropic and orthotropic nature of CNT fibers is accounted despite the fact that CNTs have one dimension in nano range and possess high stiffness only in axial direction. TABLE 1 shows the properties of CNTs that are adopted in this analysis for modeling of CNT as continuum material.

Even the CNT structure is considered as a hollow cylinder, in continuum modeling of CNT, a solid cylindrical tube with equivalent volume fraction can be considered as shown in Figure 2.

TABLE 1 : Material properties of carbon nanotubes[2]

Isotropic properties	Orthotropic properties
E_1 =1000GPa ν =0.3	E_1=1000Gpa E_2=E_3=30GPa G_{12}=G_{23}=G_{31}=30GPa ν_{12}=ν_{23}=ν_{31}=0.068

Interphase between polymer matrix/CNT

CNTs are chemically bonded structures that create the problem in interaction in between polymer matrix and themselves. This weak interaction is responsible for interphase which plays an important role in finding out the mechanical behaviour of CNT-reinforced polymer composites. Many research works are going on recently to reduce the interphase region between CNT/ polymer resin using functionalized CNTs, but it is very difficult to remove the interphase. It therefore becomes necessary to model the interphase with separate properties. In available literature many techniques have been applied for modeling of interphase[2,11,14] that gives insight view for consideration of interphase. In present work, interphase is modeled as a continuous media with isotropic properties depending on the properties of polymer. Two types of interphases considered are: rigid or stiff (where isotropic elastic modulus $E_{int} \approx 10E_m$) and soft (in which $E_{int} \approx E_m/10$).

FINITE ELEMENT ANALYSIS OF RVE

In CNT reinforced polymers, the overall composite behave like an orthotropic material. In this analysis, transversely isotropic properties are considered for estimating the stiffness matrix and elastic constants. CNT fibers and matrix are considered to be perfectly bonded at the interphase. For transversely isotropic material, five independent elastic constants (E_1, E_2, $\nu_{23,}$ ν_{12} and G_{12}) are needed to find out the material behavior[18]. Out of above effective material constants, the constants namely elastic moduli E_1, E_2 and Poisson's ratio ν_{23} related to normal stress and strain components are ob-

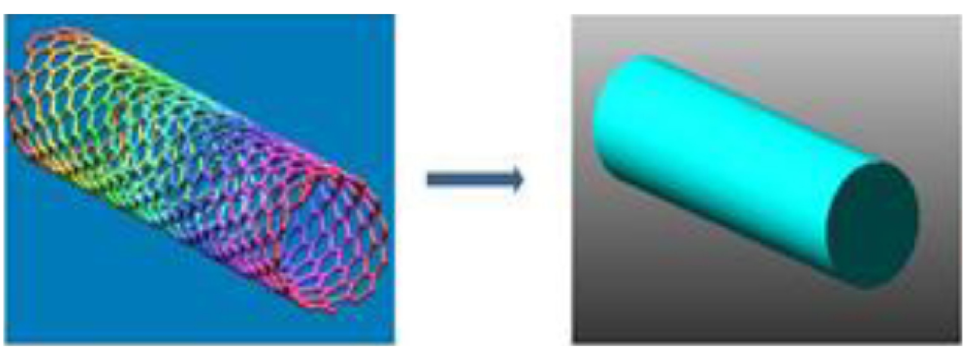


Figure 2 : Continuum model of a CNT

tained in this work. The inter-laminar shear modulus G_{23} can be also computed as function of transverse elastic modulus E_2. The general stress–strain relations for the normal stresses and strains in a transversely isotropic material can be written as:

$$\begin{Bmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\end{Bmatrix}=\begin{bmatrix}C_{11} & C_{12} & C_{12}\\ C_{12} & C_{22} & C_{23}\\ C_{12} & C_{23} & C_{33}\end{bmatrix}\begin{Bmatrix}\varepsilon_1\\ \varepsilon_2\\ \varepsilon_3\end{Bmatrix} \quad (5)$$

Here, the direction 1 refers to the longitudinal axis of fibres. The constants C_{11}, C_{12},… are obtained by applying following three different load cases: (i) A unit strain is applied along direction-1 (z-axis) and measure the first column elements of the C matrix above (ii) A unit strain is applied along direction-2 (x-axis) and measure second column elements of C and (iii) apply unit strain along direction-3 (y-axis) and measure third column elements of matrix C. Along with unit strain, the following displacement boundary conditions are also applied to first load case (as in Figure 1b):

$$\begin{aligned}&u_1(a_1, y, z) = a_1\\ &u_1(0, y, z) = 0\\ &u_2(x, a_2, z) = 0\\ &u_2(x, 0, z) = 0\\ &u_3(x, y, a_3) = 0\\ &u_3(x, y, z) = 0\end{aligned} \quad (6)$$

The average stress field (σ_α) giving the required component of elastic matrix for first load case is defined as:

$$C_{\alpha 1} = \sigma_\alpha = \frac{1}{V}\int_V \sigma_\alpha(x, y, z)dV \quad (7)$$

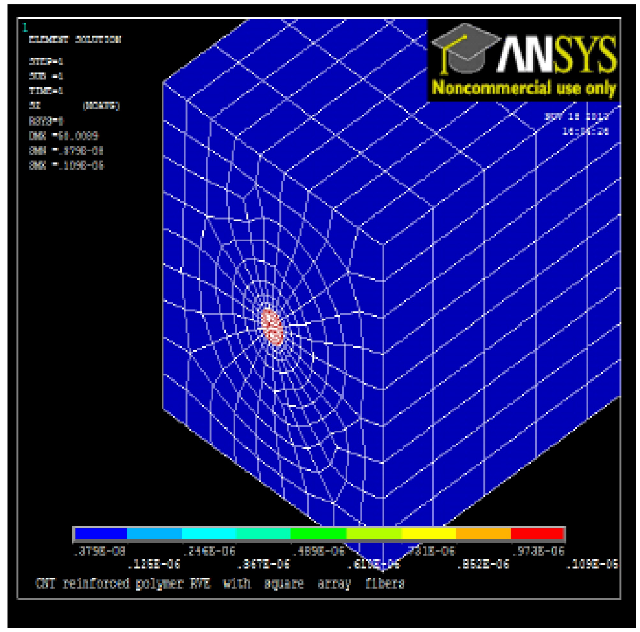
Similar boundary conditions are applied for second and third load cases. Finally, using the elements of C matrix, the elastic modulus and Poisson's ratio are obtained as:

$$\begin{aligned}&E_{C1} = C_{11} - 2C^2_{12}/(C_{22} + C_{23})\\ &E_{C2} = E_{C3} = [C_{11}(C_{22} + C_{23}) - 2C^2_{12}](C_{22} - C_{23})/(C_{11}C_{22} - C^2_{12})\\ &\nu_{C23} = [C_{11}C_{23} - C^2_{12}]/(C_{11}C_{22} - C^2_{12})\\ &G_{C23} = (C_{22} - C_{23})/2\end{aligned} \quad (8)$$

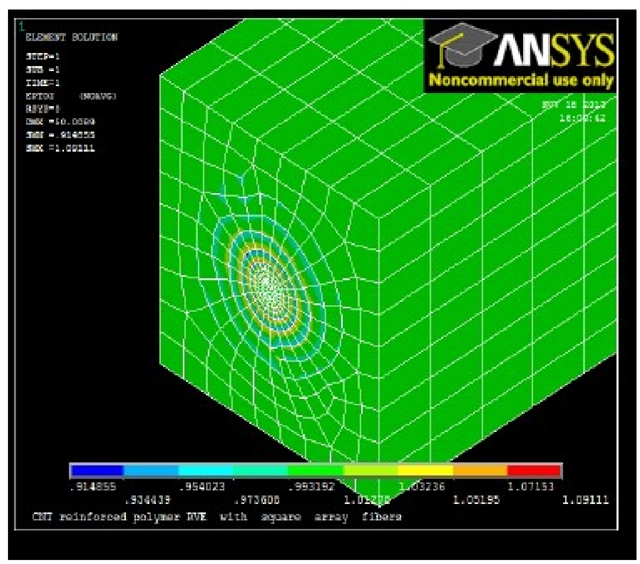
The validation of finite element model has been checked through a comparison with rule of mixture results. Prediction of elastic constant for RVE of transversely orthotropic composite is done for different volume fractions.

RESULTS AND DISCUSSION

All the three phases of the solid model of RVE are meshed with 8-noded three dimensional SOLID185 elements in ANSYS. The average stress and strain distribution for loading in direction-1 with 1% volume fraction of orthotropic CNTs is shown in Figure 3.



(a) Average stresses



(b) Average strains

Figure 3 : Average distribution plots in ANSYS model for 1% volume fraction of CNTs

An ANSYS-APDL command list is employed to carry-out parametric studies. Both the fiber volume fraction and interphase thickness are varied and corresponding the elastic constants are recorded. TABLE 2 shows the results of analytical approach with those obtained from FEM for 1% volume fraction of CNT. Also shown are the results for the case accounting the interphase elasticity effect corresponding to 0.34nm thickness of interphase.

TABLE 2 : Elastic constant obtained for CNT-reinforced polymer with an interphase

Elastic Constant	Analytical result	FEM result		FEM result with interphase	
		Isotropic CNT	Orthotropic CNT	Stiff	soft
E_{C1}(GPa)	12.4749	13.927	14.270	15.267	13.908
E_{C2}(GPa)	2.5251	2.765	2.751	2.827	2.572
G_{C23}(GPa)	0.9419	0.9484	0.9467	0.9523	0.8964
ν_{C23}	0.3396	0.4575	0.4567	0.4556	0.4357

It is seen that the analytical results as computed from rule of mixture are always on the lower side and by considering stiff interphase conditions the elastic constants have attained maximum values. Figure 4 shows the variation of longitudinal modulus (E_{C1}) with volume fraction of CNT. It is seen that the variation is almost identical in two cases when CNT behavior is considered as orthotropic and isotropic in nature. Although FEM results are in good agreement with rule of mixture, but they show deviation from Halpin-Tsai model. It is because of the assumption made in FEM modeling that all phases are considered as continuum and neglected the reinforcing efficiency parameter between CNT and polymer.

Figures 5 to 7 show the variation of inter-laminar shear modulus (Gc_{23}), transverse modulus (E_{C2}) and Poisson ratio (ν_{C23}) with CNT volume fractions. It is concluded that these properties are less affected by accounting orthotropic nature of CNT.

The effect of interphase thickness and stiffness is studied first to confirm whether the role of interphase during the modeling of CNT reinforced polymer composites. Study is made for rigid (stiff) interphase because such an interphase gives maximum elastic properties in comparison to soft interphase as reveled from TABLE 2. The minimum thickness of interphase considered for this investigation is equal the CNT thickness (=0.34nm) and results are estimated by varying the ratio of interphase thickness with CNT thickness. Figure 8 shows the variation longitudinal elastic modulus (E_{c1}) with the interphase thickness for different volume fractions.

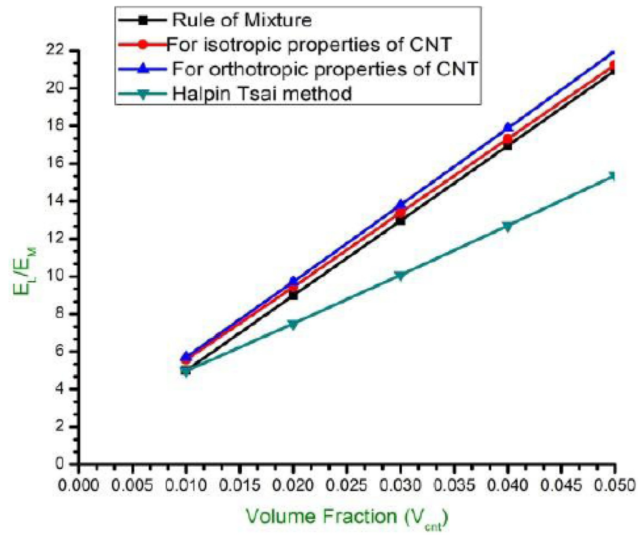


Figure 4 : Variation of longitudinal modulus with CNT volume fraction

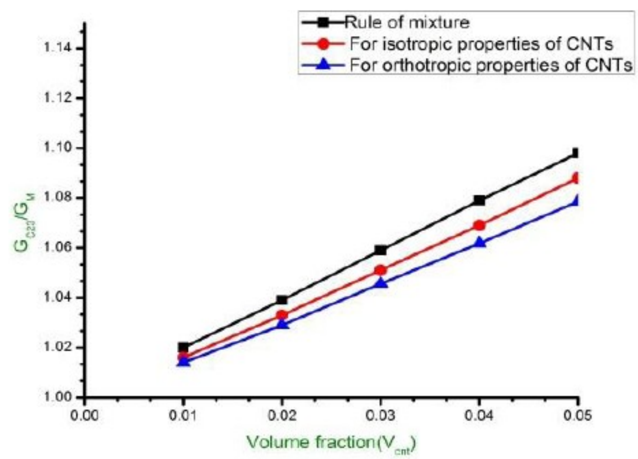


Figure 5 : Variation of interlaminar shear modulus with volume fraction

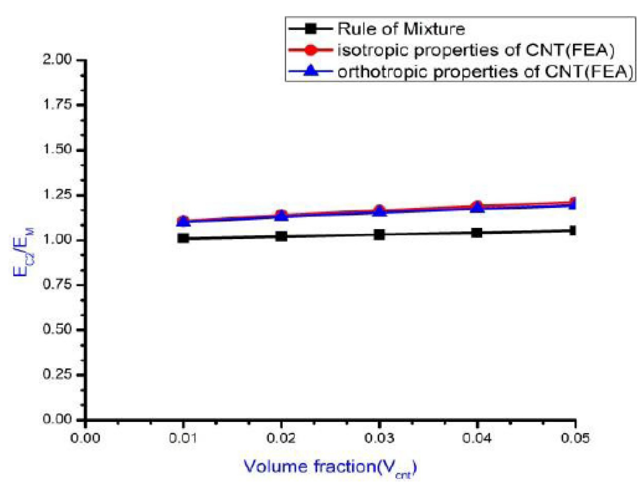


Figure 6 : Variation of transverse modulus with volume fraction

The first important conclusion is that longitudinal modulus is less affected by the interphase thickness in

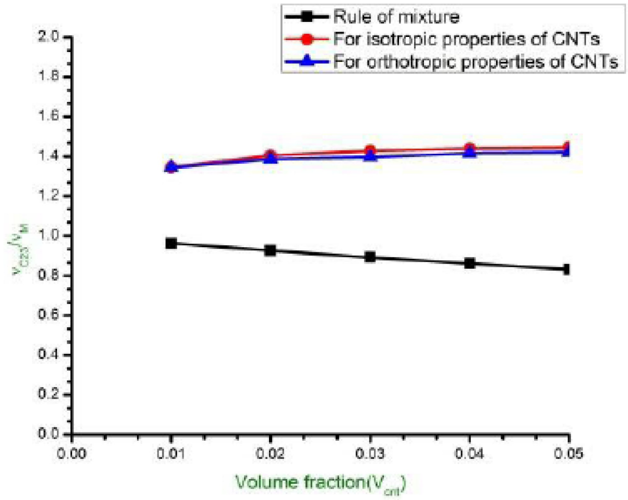


Figure 7 : Variation of Poisson's ratio with volume fraction

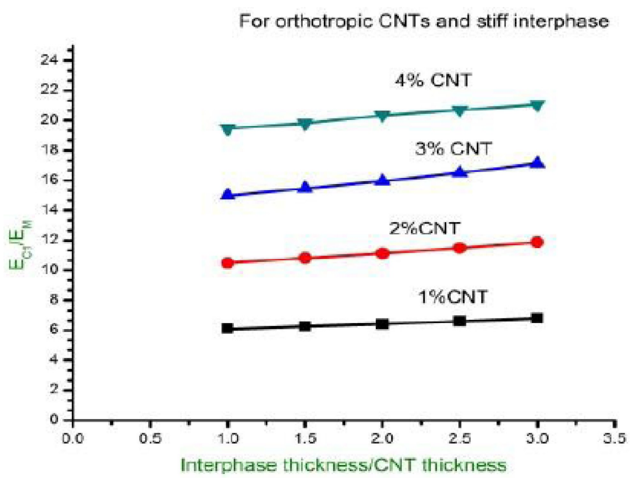


Figure 8 : Effect of interphase thickness on longitudinal modulus

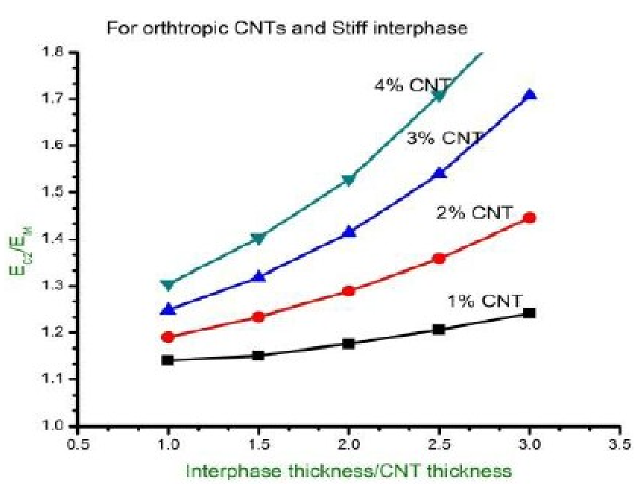


Figure 9 : Effect of interphase thickness on transverse modulus

comparison to transverse modulus for all volume fractions. Thus, for simplicity, interphase effect can be neglected in estimating of longitudinal elastic modulus. On the other hand, interphase stiffness and thickness affects transverse modulus and other polymer matrix dominated properties as shown in Figures 9 and 10.

Figure 11 shows the variation of Poisson's ratio with interphase thickness and it seems that interphase thickness has adverse effect on out of plane Poisson's ratio.

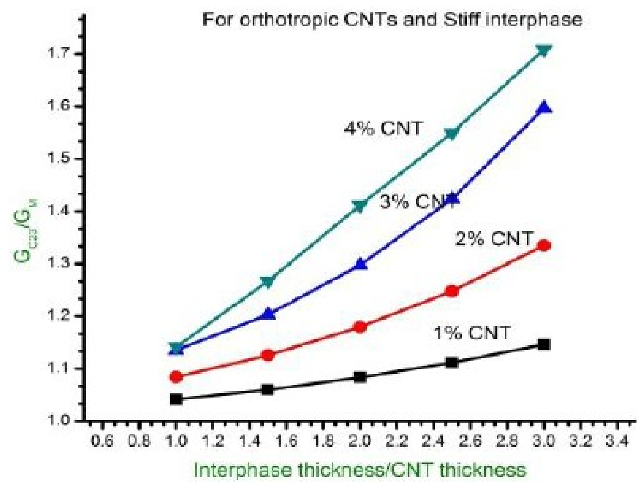


Figure 10 : Effect of interphase thickness on inter laminar shear modulus

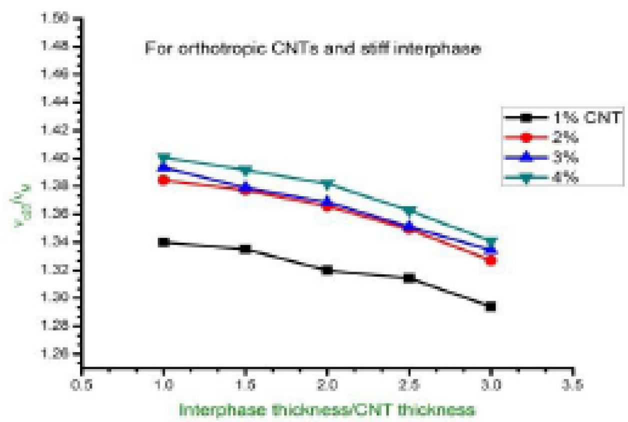


Figure 11 : Effect of interphase thickness on Poisson's ratio

CONCLUSION

In present work, computational approach based on finite element analysis has been illustrated to predict the effective transversely isotropic properties of CNT-reinforced composites. A homogenized RVE consisting of polymer resin, single walled carbon nanotube and an interphase with proper boundary conditions was analyzed using three-dimensional finite element analysis. During the parametric studies, the effects of parameters such as volume fraction, interphase stiffness and thickness were considered. Both orthotropic and isotropic material properties have been separately accounted in this investigation. It is concluded that the interphase effect is mostly on transverse elastic properties rather than in longitudinal direction. Hence, if enhancement in longitudinal elastic modulus is desirable then there is no need to improve interphase property. Moreover, interphase effect can be neglected in evaluation of longitudinal elastic modulus.

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